

Deformations and quasiparticle spectra of nuclei in the nobelium region

Yue Shi,^{1,2,3} J. Dobaczewski,^{3,4} P.T. Greenlees,³ J. Toivanen,³ and P. Toivanen,³

¹*Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA*

²*Physics Division, Oak Ridge National Laboratory, Post Office Box 2008, Oak Ridge, Tennessee 37831, USA*

³*Department of Physics, PO Box 35 (YFL), FI-40014 University of Jyväskylä, Finland*

⁴*Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, ul. Hoża 69, PL-00681 Warsaw, Poland*

We have performed self-consistent Skyrme Hartree-Fock-Bogolyubov calculations for nuclei close to ^{254}No . Self-consistent deformations, including $\beta_{2,4,6,8}$ as functions of the rotational frequency, were determined for even-even nuclei $^{246,248,250}\text{Fm}$, $^{252,254}\text{No}$, and ^{256}Rf . The quasiparticle spectra for $N = 151$ isotones and $Z = 99$ isotopes were calculated and compared with experimental data and the results of Woods-Saxon calculations. We found that our calculations give high-order deformations similar to those obtained for the Woods-Saxon potential, and that the experimental quasiparticle energies are reasonably well reproduced.

Keywords: Self-consistent mean-field calculations; self-consistent deformations; quasiparticle energies.

1. Introduction

Nuclei in the nobelium region represent the heaviest systems for which detailed spectroscopic information on the structure is available.¹ Hence, they provide an excellent testing ground for various theoretical models that aim at reliable predictions of properties of superheavy elements. Although significant progress has been made both experimentally and theoretically, there are still challenges for self-consistent mean-field calculations (see Ref. 2 for a recent review). One of the challenges is the correct description of deformed shell gaps. Macroscopic-microscopic calculations predict shell gaps at $N = 152$ and $Z = 100$, whereas typical self-consistent mean-field calculations give shell gaps at $N = 150$, and $Z = 98$ and $Z = 104$. The experimental findings are consistent with the macroscopic-microscopic shell

gaps.

Current advanced readjustements³ of coupling constants of the Skyrme functional do not cure this deficiency, although they point to a large under-determination of the spin-orbit properties. To study detailed spectroscopic properties of heavy and superheavy nuclei, one thus may attempt a fine tuning of the spin-orbit coupling constants, so as to bring the deformed shell gaps in closer agreement with data. For this purpose, we recently readjusted⁴ the spin-orbit coupling constants, $C_0^{\nabla J}$ and $C_1^{\nabla J}$, and pairing strengths, V_0^ν and V_0^π , of the Skyrme UNEDF1 functional³ to match the experimental excitation energies of the $11/2^-$ state in ^{251}Cf and $7/2^+$ state in ^{249}Bk . For the time-odd coupling constants of the functional, we adopted the prescription based on the Landau parameters, as defined in Ref. 5. The remaining parameters of UNEDF1 were kept unchanged. We call this new parameter set UNEDF1_L^{SO}. Details of the adjustment procedures will be presented in a forth-coming publication.⁴ Here we only quote the obtained values, which read,

$$(C_0^{\nabla J}, C_1^{\nabla J}) = (-88.05040, 8.45838) \text{ MeV fm}^5, \quad (1)$$

$$(V_0^\nu, V_0^\pi) = (-205.05, -252.48) \text{ MeV}. \quad (2)$$

As a result, in Ref. 4 we found improvements of shell gaps, quasiparticle energies, and moments of inertia (MoI) in nuclei around ^{254}No . Also a good agreement with experiment has been obtained for the quasiparticle energies in ^{249}Bk and ^{251}Cf . The single-particle spectra more closely resemble those obtained with the WS potential, and shell gaps are opened at $Z = 100$ and $N = 152$ in ^{254}No . In the present work, we extended the calculations to other nuclei in the nobelium region. We investigated the self-consistent deformations as a function of frequency and we performed blocked calculations for odd- A $N = 151$ isotones and Es ($Z = 99$) isotopes.

2. The model

In this work, all the calculations were performed by using the symmetry-unrestricted solver HFODD⁶ (v2.52j). For rotational calculations, the standard cranking term $-\omega J_y$ was added to the Hamiltonian. The effect of an odd nucleon was treated by employing the blocking approximation, that is, by using the density matrix and pairing tensor in the form,⁷

$$\rho_{mn}^\mu = (V^* V^T)_{mn} + U_{m\mu} U_{n\mu}^* - V_{m\mu}^* V_{n\mu}, \quad (3)$$

$$\kappa_{mn}^\mu = (V^* U^T)_{mn} + U_{m\mu} V_{n\mu}^* - V_{m\mu}^* U_{n\mu}. \quad (4)$$

We refer the reader to Ref. 8 for details.

In the cranking-plus-blocking calculations, the time-reversal symmetry is broken, so the time-odd terms of the Skyrme density functional are present. The importance of time-odd terms in describing collective rotational bands has been emphasized in Ref. 9. The advantage of using a symmetry-unrestricted solver is that the effects of non-zero time-odd potentials can be taken into account in a strict manner.

We used 680 deformed harmonic-oscillator basis states, with the basis-deformation parameters of $\hbar\omega_x = \hbar\omega_y = 8.5049\text{ MeV}$ and $\hbar\omega_z = 6.4823\text{ MeV}$. The cutoff energy in the quasiparticle spectrum was $E_c = 60\text{ MeV}$. In the pairing channel, to describe the approximate particle-number projection, we adopted the Lipkin-Nogami formalism.

3. Results

In the nobelium region, high-order deformations of the WS potential were found to play important roles in explaining many high-spin phenomena. For example, the decrease of $E_x(2^+)$ in $^{254}\text{No}^{10}$ and the delayed upbending of MoI in ^{254}No as compared to $^{252}\text{No}^{11}$ were attributed to the effect of β_6 deformation on the relevant single-particle levels.

We performed cranking calculations for the 6 nuclei, in which the ground-state rotational bands are observed, namely, for $^{246,248,250}\text{Fm}$, $^{252,254}\text{No}$, and ^{256}Rf . We determined the MoIs, proton and neutron pairing gaps, and self-consistent deformations as functions of the rotational frequency.⁴ The experimental kinematic and dynamic MoIs were well reproduced by our calculations. Deformations obtained within our fully self-consistent calculations provide a reasonable description of polarization effects exerted by the occupations of individual deformed orbitals. They were determined as the Bohr deformation parameters β_λ of sharp-edge mass distributions that have multipole moments Q_λ , for $\lambda = 2-8$, identical to those calculated microscopically, see Ref. 12. All nuclei considered here have axial ground-state shapes.

Figure 1 shows deformations $\beta_{2,4,6,8}$ as a function of rotational frequency ω . At $\omega = 0$, deformations β_2 are systematically higher than those obtained by macroscopic-microscopic WS calculations,^{10,11} and, in general, lower than those obtained within other relativistic and non-relativistic mean-field calculations.^{13,14} It is interesting to note that the high-order deformations presented in Figure 1 are very close to those of Refs. 10 and 11. With increasing rotational frequency, the deformations stay almost constant. Only at $\omega \sim 0.3\text{ MeV}$, deformations β_2 begin to decrease. This behavior is consistent with that of Ref. 11.

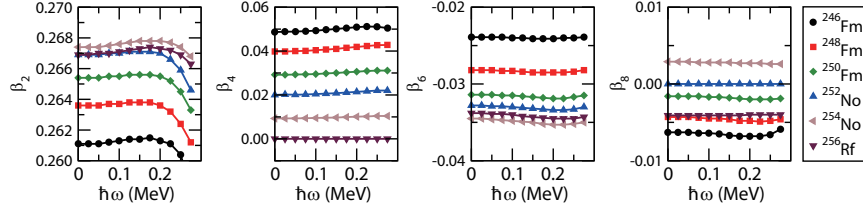


Fig. 1. Deformations $\beta_{2,4,6,8}$ as functions of the rotational frequency, calculated self-consistently for six nuclei, $^{246,248,250}\text{Fm}$, $^{252,254}\text{No}$, and ^{256}Rf .

Figure 2 (left) shows the calculated quasiparticle spectra for $N = 151$ isotones from $Z = 94$ to 104. For these nuclei, experimental data are available in this mass region.¹⁵ The observed ground states are dominated by the $9/2[734]$ orbital, with the $5/2[622]$ state located at ~ 200 keV. In ^{245}Pu and ^{247}Cm , our calculations predict ground states of $9/2[734]$. For heavier isotones, the $7/2[624]$ state becomes lower than the $9/2[734]$ state, but only by several tens of keV. These two levels are right below the $N = 152$ shell gap. They are very close to each other, and change order with increasing proton number. This indicates that (i) there is a significant N -dependence of the single-particle and quasiparticle energies and (ii) adjusting the spin-orbit force to obtain better agreement for the $11/2^-$ state in ^{251}Cf results in the $j_{15/2}$ and $g_{9/2}$ spherical shells being too close together. The present calculations predict a $5/2[622]$ state which is too high and underestimate the energies of the $7/2[624]$ and $1/2[620]$ states.

Comparing our results with those of Ref. 16, we note the presence of low-lying $7/2[624]$ states there too. We also note an overestimation of their $1/2[620]$ energies. The excitation energy of the $1/2[620]$ orbital is related to the shell gap at $N = 152$. Its isospin dependence is very interesting – we note that our results reproduce the observed increase of excitation energy of $1/2[620]$ with increasing proton number.¹⁵

Experimental information on quasi-proton spectra are relatively scarce.¹ Close to $Z = 100$, systematic spectra are only observed for Es ($Z = 99$) isotopes.¹⁷ Figure 2 (right) displays the calculated quasiparticle spectra for $Z = 99$ isotopes from $N = 144$ to 154. One can see that for the ground states the calculations predict two very close states, $3/2[521]$ and $7/2[633]$, which is consistent with experimental observations.¹⁷ Compared to the calculations presented in Ref. 17, our results show a much lower $3/2[521]$ orbital. This is because our calculations predict very close $7/2[633]$ and $3/2[521]$ levels below the $Z = 100$ shell opening, whereas the WS calculations give them

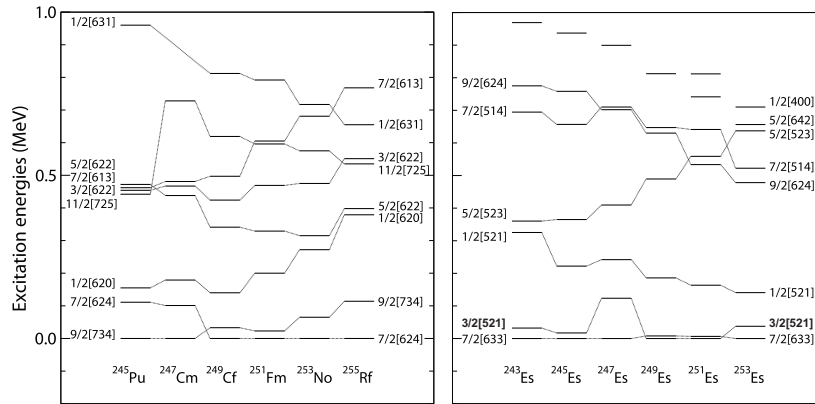


Fig. 2. Quasiparticle energies calculated for the UNEDF1 $_L^{\text{SO}}$ parameter set,⁴ and for the $N = 151$ isotones (left) and Es ($Z = 99$) isotopes (right).

~ 200 keV apart. The $7/2[514]$ state is also systematically observed in the Es isotopes. However, our calculation fails to reproduce the increase of excitation energy of this orbital with increasing neutron number. We also note that in our calculations, the $5/2[523]$ states exhibit an increase similar to that observed in experiment for the state attributed to the $7/2[514]$ orbital. Further experimental and theoretical work is needed for these odd- Z nuclei.

4. Conclusion

We performed self-consistent Skyrme Hartree-Fock-Bogolyubov calculations for nuclei in nobelium region. Deformations $\beta_{2,4,6,8}$ were studied for even-even nuclei $^{246,248,250}\text{Fm}$, $^{252,254}\text{No}$, and ^{256}Rf . The quasiparticle spectra for $N = 151$ isotones and $Z = 99$ Es isotopes were systematically calculated by using the blocking approximation within the Hartree-Fock-Bogolyubov method. Comparisons were made with the available experimental data and WS calculations. It was found that our results give similar deformations to those obtained within the WS calculations. The observed quasi-particle energies are reasonably well reproduced, especially for proton quasiparticle states.

Acknowledgments

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